IgMinRESEARCH A BioMed & Engineering Journal
Focusing on Biology, Medicine and Engineering disciplines
BIOLOGY ISSN 2995-8067
Chemistry | Applied Science | Biochemistry

Article Information

Submitted: November 13, 2023
Approved: November 20, 2023
Published: November 21, 2023

How to cite this article: Undalov Yu K. Homologous Series of Chemical Compounds in Three-component Systems ($A^{a+} - B^{b+} - C^{c-}$) and (Zn^{2+} - Ge^{4+} - P^{3-}) in Generalized Form. IgMin Res. Nov 21, 2023; 1(1): 060-069. IgMin ID: igmin117; DOI: 10.61927/igmin117; Available at: www.igminresearch.com/articles/pdf/igmin117.pdf

Keywords: Homological series: Chemical compounds: Charged clusters: Calculation method: Three-component systems

Check for updates

Research Article

Homologous Series of Chemical Compounds in Three-component Systems ($A^{a+} - B^{b+} - C^{c-}$) and (Zn^{2+} - Ge^{4+} - P^{3-}) in Generalized Form

Undalov Yu K*

Ioffe Institute of the Russian Federation Academy of Sciences, Saint-Petersburg, Russia

***Correspondence:** Undalov Yu K, Ioffe Institute of the Russian Federation Academy of Sciences, Saint-Petersburg, Russia, Email: undal@yandex.ru

Abstract

For the first time, a method for calculating formulas of homologous series of chemical compounds of the systems ($A^{a+} - B^{b+} - C^{c-}$) and {$Zn^{2+} - Ge^{4+} - P^{3-}$} in a generalized form is presented. The calculation is confirmed by the literature experimentally obtained compounds: thirteen compounds of the system ($Na^{+} - Ti^{4+} - O^{2-}$), seven – systems ($Li^{+} - Ti^{4+} - O^{2-}$), five – systems ($K^{+} - V^{5+} - O^{2-}$), eight – systems ($Ba^{2+} - Cu^{2+} - O^{2-}$). Homological series in ($A^{a+} - B^{b+} - C^{c-}$) have the following generalized form: $A_{\{t-k\cdot r+nr-\eta\}bc}B_{rac}C_{\{t-k\cdot r+n\eta\}ab}$ and $A_{fbc}B_{\{r-k\cdot t+nt-\eta\}ac}C_{(r-k\cdot t+n\eta)ab}$.

In ($Zn^{2+} - Ge^{4+} - P^{3-}$) systems for the *m*-group the formulas of homologous series, that develops towards Ge_3P_4, have the following generalized form: $Zn_{6t}Ge_{(6r-6kt+6n-6\delta)}P_{(8r-8kt+8n)}$ and for αm-homologous series – $Zn_6Ge_{3n}P_{4(n+1)}$. A method for calculating formulas of homologous series of chemical compounds in a generalized form can be used for any system of chemical elements.

INTRODUCTION

The search for new Chemical Compounds (CC) in multicomponent systems of Chemical Elements (CE) is a difficult task. The great variety of properties of a set of Three-Component Chemical Compounds (TCC) is of great interest in solving a number of scientific and applied studies. There are known works in the literature that use the mathematical apparatus for predicting phases in multicomponent systems. Thus, semiempirical quantum-chemical methods, such as Hartree-Fock-Rutaan and Hartree-Fock-Slater methods [1-3], are used to calculate the formulae of hypothetical multicomponent CC. When using these methods to describe a chemical system, many physical and chemical phenomena must be taken into account. The exact solution of the basic laws leads to overcomplicated calculations. Therefore, for practically all CE systems, the solution of the corresponding electronic equations used in quantum-chemical calculations is only possible approximately. Well-known quantum-chemical methods of calculation, allow to calculate the formula of any CC, are rather complicated and require special knowledge in the field of mathematical programming.

According to the works [4-7], knowledge of the laws of formation of Homological Series (HS) of chemical compounds can be included in the process of searching for new CC.

Thus, the author of the work [8, p. 190] believes that "...the activated complex theory consists in the fact that in the course of any chemical reaction, the initial configuration of atoms passes to the final one as a result of continuous change of interatomic distances", which is characterized by the formation of various critical intermediate configurations, i.e. activated complexes". On the basis of this idea, in the works [4-7] the method of calculation of formulae of HS of chemical compounds of three-component systems of CE ions was developed.